2,3,4-Trimethylpentanoic acid

Inchi: InChI=1S/C8H16O2/c1-5(2)6(3)7(4)8(9)10/h5-7H,1-4H3,(H,9,10)
InchiKey: RWJKYJZSUKHVAN-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CC(C)C(C)C(C)C(=O)O
Mol. weight [g/mol]: 144.21
CAS: 90435-18-0

Physical Properties

Property code	Value	Unit	Source
gf	-256.58	kJ/mol	Joback Method
hf	-489.10	kJ/mol	Joback Method
hfus	11.59	kJ/mol	Joback Method
hvap	55.66	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.999		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	527.17	K	Joback Method
tc	706.01	K	Joback Method
tf	245.67	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.36	J/mol×K	527.17	Joback Method
cpg	363.68	J/mol×K	676.20	Joback Method
cpg	354.00	J/mol×K	646.40	Joback Method
cpg	343.85	J/mol×K	616.59	Joback Method
cpg	333.20	J/mol×K	586.78	Joback Method
cpg	322.04	J/mol×K	556.98	Joback Method
cpg	372.88	J/mol×K	706.01	Joback Method
dvisc	0.0001246	Pa×s	527.17	Joback Method
dvisc	0.0002230	Pa×s	480.25	Joback Method

dvisc	0.0004529	Pa×s	433.34	Joback Method
dvisc	0.0010926	Pa×s	386.42	Joback Method
dvisc	0.0033621	Pa×s	339.50	Joback Method
dvisc	0.0148357	Pa×s	292.59	Joback Method
dvisc	0.1154082	Pa×s	245.67	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90435180&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume